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Title: Uncertainty Analysis for a Criticality Benchmark

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Uncertainty Analysis for a Criticality Benchmark

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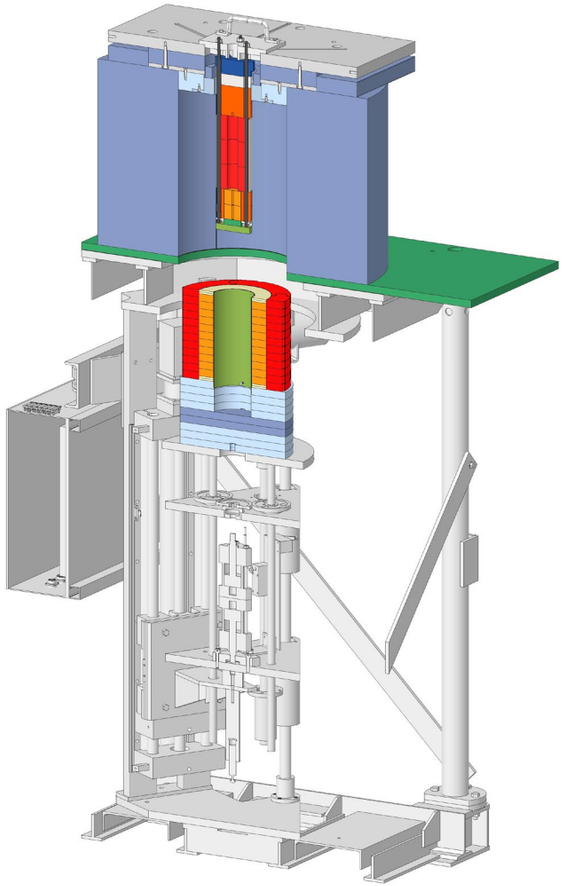
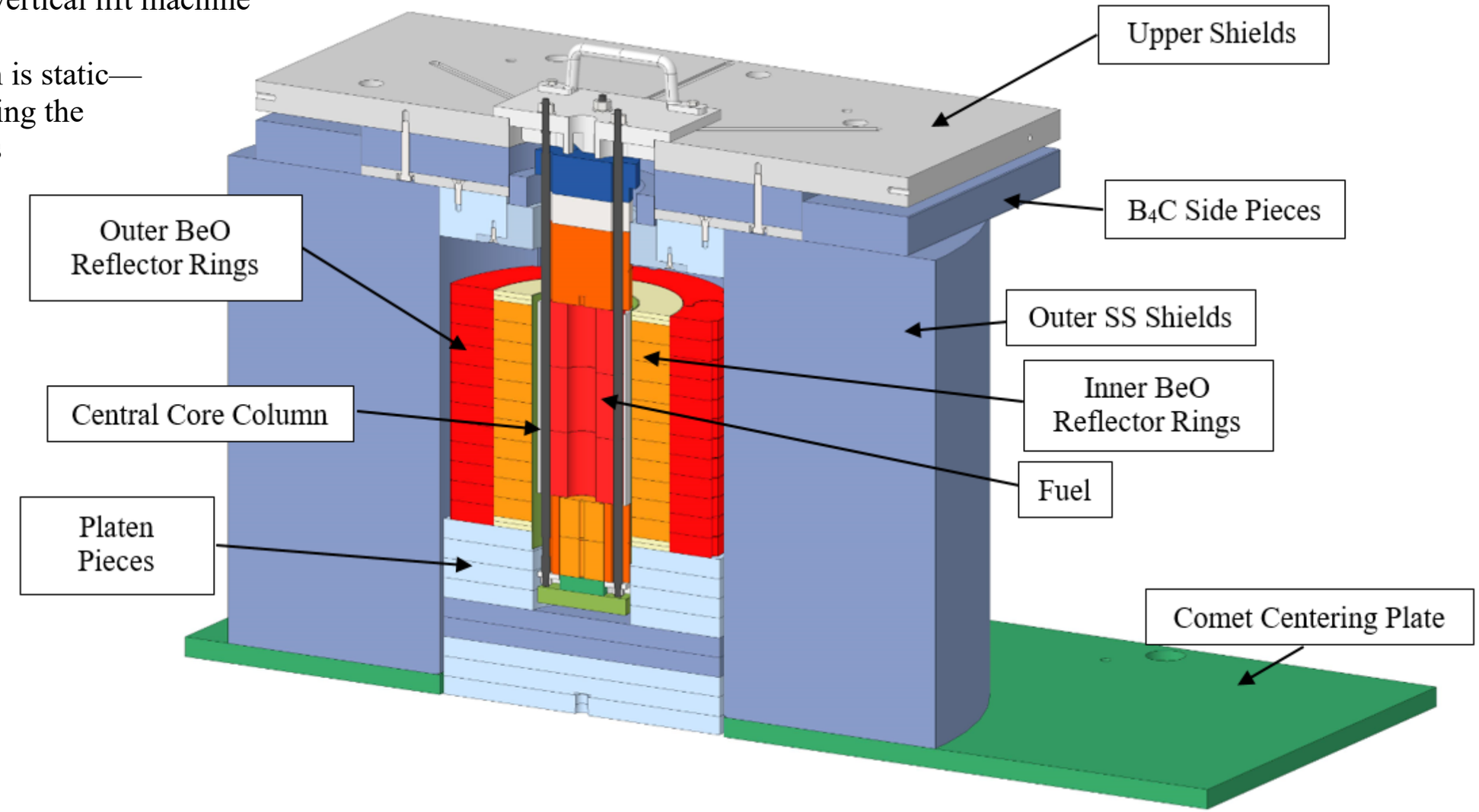
CONNECT
March 1, 2021

Kilopower Reactor Using Stirling Technology (KRUSTY)

- Installed on the Comet vertical lift machine
- The central core column is static—criticality is achieved by raising the platen and the BeO reflectors



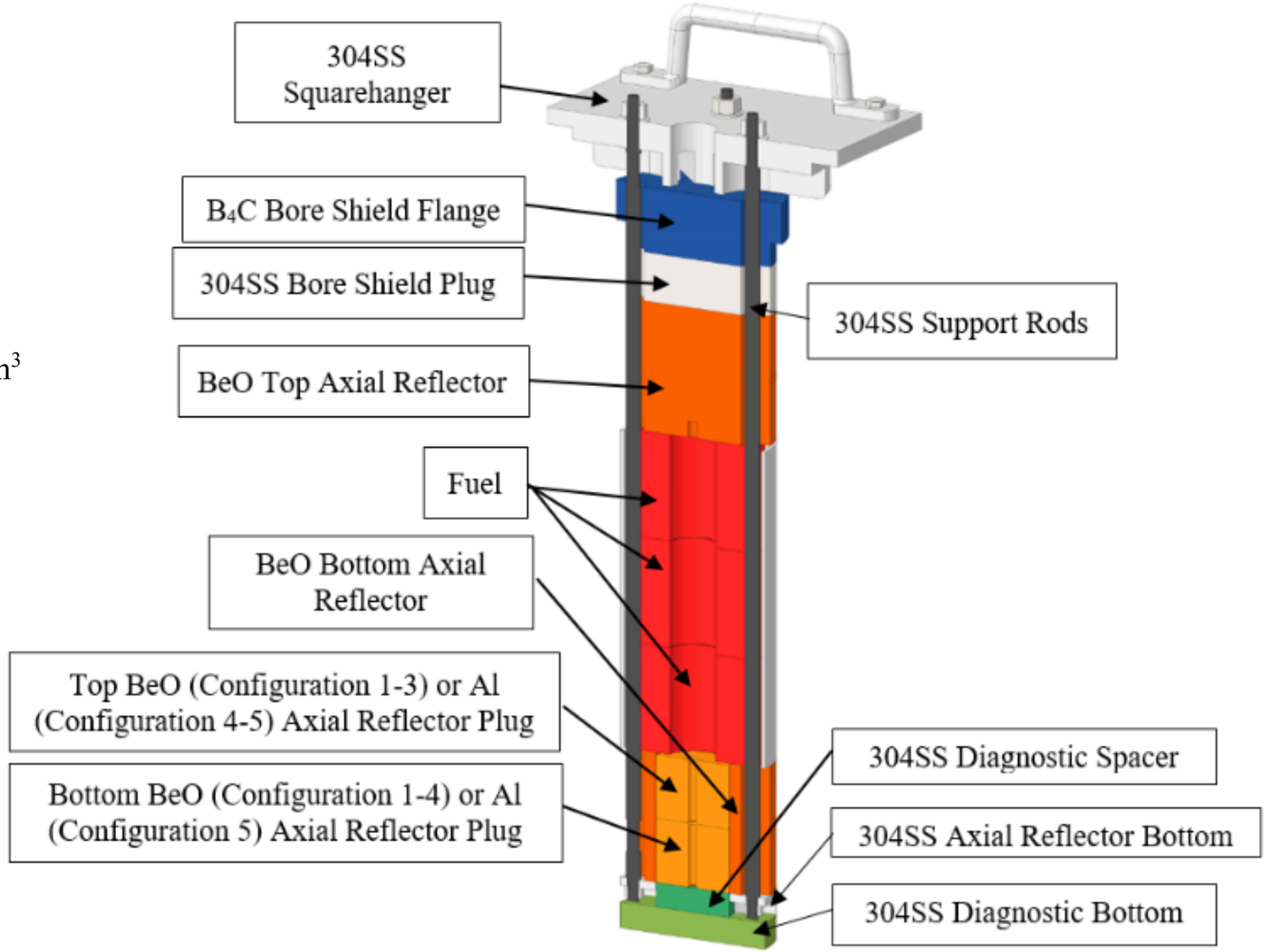


Central Core Column

- 32.200 kg of fuel:
highly enriched uranium (HEU)
+ 7.65 wt% molybdenum

- 93.1 wt% U-235

- Average fuel density was 17.34 g/cm^3



Neutron Transport

- We analyzed KRUSTY with LANL's MCNP neutron transport code.
  + Monte Carlo N-Particle

- In the Monte Carlo method, neutrons are born in fission events and fly around the geometry having events (e.g., scatter, capture, fission, escape) according to the natural probabilities.

- "Natural probabilities" are given as *neutron cross sections*, which are measured and evaluated nuclear data.

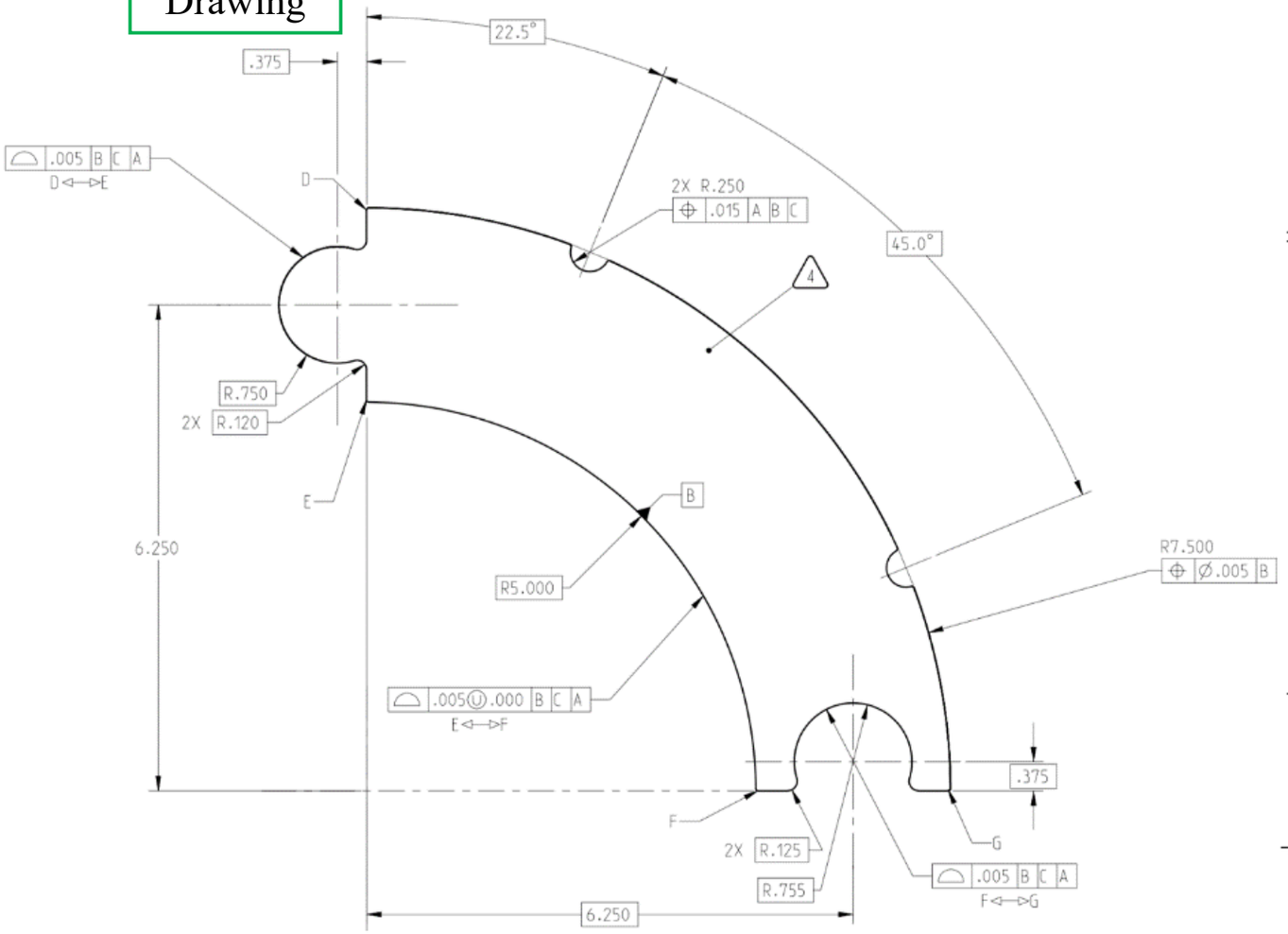
- One of the goals of the benchmark project is to improve the nuclear cross sections (and the codes that use them).

- In this work, the response of interest is called k_{eff}, which describes the neutron multiplication in a near-critical system:
  + $k_{eff} = 1$ means the system is self-sustaining (losses balance production) and the neutron population is stable
  + $k_{eff} < 1$ means the system is subcritical and neutron chains will die out; the neutron population decreases with time
  + $k_{eff} > 1$ means the system is supercritical and the neutron population increases with time
  + $k_{eff} > 1.00640$ means the system is VERY supercritical

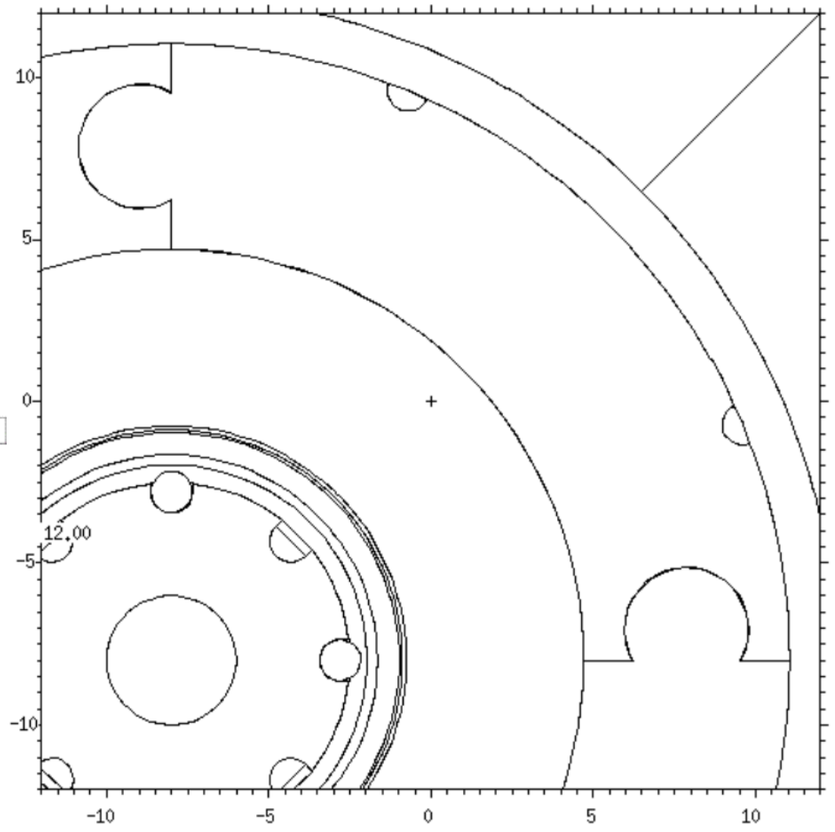
- Like most quantities we all care about, k_{eff} is not measured directly; it is only inferred.

Outer BeO Radial Reflector

Drawing



MCNP Model



Why?

- To develop a benchmark with which to evaluate neutron transport codes and (especially!) data.

- "The ICSBEP Handbook now includes data for 582 evaluations containing acceptable benchmark specifications for 5,053 critical, subcritical, or near-critical configurations, representing contributions from 23 countries." (Bess et al., *TANS* **123**, 2020)

- A major effort of the benchmark process is to evaluate the uncertainty of the experiment.

Uncertainty Quantification

- The variance in a response k due to uncertainty in parameter x is $\left(u_k\right)^2 = \left(\frac{\partial k}{\partial x}\right)^2 \left(u_x\right)^2$
- More generally, $\left(u_k\right)^2 = \left(\frac{\partial k}{\partial x_1}\right)^2 \left(u_{x_1}\right)^2 + \left(\frac{\partial k}{\partial x_2}\right)^2 \left(u_{x_2}\right)^2 + \cdots + \left(\frac{\partial k}{\partial x_N}\right)^2 \left(u_{x_N}\right)^2$

$$= \sum_{n=1}^{N} \left(\frac{\partial k}{\partial x_n}\right)^2 \left(u_{x_n}\right)^2$$

- Still more generally, $\boxed{\left(u_k\right)^2 = \underline{S}^T \underline{\underline{C}} \underline{S}}$ (the Sandwich Formula) where

$\underline{S}^T = \begin{bmatrix} \frac{\partial k}{\partial x_1} & \frac{\partial k}{\partial x_2} & \cdots & \frac{\partial k}{\partial x_N} \end{bmatrix}$ is the vector of sensitivities

$\underline{\underline{C}} = \begin{bmatrix} \mathrm{cov}(x_1,x_1) & \mathrm{cov}(x_1,x_2) & \cdots & \mathrm{cov}(x_1,x_N) \\ \mathrm{cov}(x_2,x_1) & \mathrm{cov}(x_2,x_2) & \cdots & \mathrm{cov}(x_2,x_N) \\ \vdots & \vdots & \ddots & \vdots \\ \mathrm{cov}(x_N,x_1) & \mathrm{cov}(x_N,x_2) & \cdots & \mathrm{cov}(x_N,x_N) \end{bmatrix}$ is the covariance matrix $= \begin{bmatrix} \mathrm{var}(x_1) & \mathrm{cov}(x_1,x_2) & \cdots & \mathrm{cov}(x_1,x_N) \\ \mathrm{cov}(x_2,x_1) & \mathrm{var}(x_2) & \cdots & \mathrm{cov}(x_2,x_N) \\ \vdots & \vdots & \ddots & \vdots \\ \mathrm{cov}(x_N,x_1) & \mathrm{cov}(x_N,x_2) & \cdots & \mathrm{var}(x_N) \end{bmatrix}$

Uncertainty Quantification for ICSBEP Benchmarks

- $u_{k,i} = \frac{\pm u_i}{2\delta x_i}\left[k_{eff}(x_{i,0} + \delta x_i) - k_{eff}(x_{i,0} - \delta x_i)\right]$

- If you think in terms of scaling factors: $\frac{2\delta x_i}{u_i}$ is the number of standard deviations corresponding to the perturbation δx_i;

divide Δk_{eff} by that.

- If you think in terms of sensitivities,

  + $\frac{1}{2\delta x_i}\left[k_{eff}(x_{i,0} + \delta x_i) - k_{eff}(x_{i,0} - \delta x_i)\right]$ is a central-difference estimate of $\left.\frac{\partial k_{eff}}{\partial x_i}\right|_{x_i = x_{i,0}}$ and $\left(u_{k,i}\right)^2 = \left(\left.\frac{\partial k_{eff}}{\partial x_i}\right|_{x_i = x_{i,0}}\right)^2 \left(u_i\right)^2$

Inputs for a k_{eff} calculation

- Geometry (dimensions, which are material interfaces and the outer boundary)
- Materials
  + Composition
  + Density
- Neutron cross sections

Inputs for a k_{eff} ~~calculation~~ measurement

- Geometry (dimensions, which are material interfaces and the outer boundary)
- Materials
  - + Composition
  - + ~~Density~~ Mass
- ~~Neutron cross sections~~

Uncertainties are Evaluated in 6 Categories

1. Critical measurement (and inference of k_{eff})
2. Mass of each part
3. Geometry/dimensions of each part
4. Material composition of each part
5. Positioning/surroundings
6. Temperature

- Parts: 3 fuel + 68 BeO rings +4 more BeO + 6 aluminum + 10 steel (core column) + 1 B_4C (core column) + 1 AmBe source + 9 steel and B_4C (platen) + 8 outer steel + 9 steel and B_4C (upper shielding) = ~119 parts
  - + Each part has 1 mass
  - + Each part has ~3 or 4 dimensions

- 20 materials
  - + Each material has ~10–20 elements

How many transport calculations are needed for the KRUSTY uncertainty analysis (mass and composition)?

- Central-difference formula for uncertainty in k due to parameter x_i: $u_{k,i} = \frac{\pm u_i}{2\delta x_i}\left[k_{eff}(x_{i,0} + \delta x_i) - k_{eff}(x_{i,0} - \delta x_i)\right]$
- Mass of each part: 2 × ~119 parts = ~138
- Material composition of each part: 2 × 20 materials × ~10–20 elements = ~400–800
- Each one of these takes ~2½ hours

How many transport calculations are needed for the KRUSTY uncertainty analysis (mass and composition)?

- Central-difference formula for uncertainty in k due to parameter x_i: $u_{k,i} = \frac{\pm u_i}{2\delta x_i}\left[k_{eff}(x_{i,0} + \delta x_i) - k_{eff}(x_{i,0} - \delta x_i)\right]$
- Mass of each part: 2 × ~119 parts = ~138
- Material composition of each part: 2 × 20 materials × ~10–20 elements = ~400–800
- Each one of these takes ~2½ hours

- We can do all this in one calculation!

  + $S_{k,x_i} = \frac{x_{i,0}}{k_{eff,0}} \frac{\partial k_{eff}}{\partial x_i}\bigg|_{x_i = x_{i,0}}$ is output from MCNP and many other transport codes for x_i = the atom density of nuclide i
  + Takes ~ 4 hours

- Deterministic transport codes take two calculations.

ANS

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Adjoint-Based Sensitivity and Uncertainty Analysis for Density and Composition: A User's Guide

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How many transport calculations are needed for the KRUSTY uncertainty analysis (dimensions and positioning)?

- Central-difference formula for uncertainty in k due to parameter x_i: $u_{k,i} = \frac{\pm u_i}{2\delta x_i}\left[k_{eff}(x_{i,0} + \delta x_i) - k_{eff}(x_{i,0} - \delta x_i)\right]$
- Dimensions of each part: 2 × ~119 parts × 3–4= ~414–952
- Position of some components: ~2 × ~4 assemblies = ~8
- Gaps: 1 × ~80 places where there could be a gap = ~80
- Each one of these takes ~2½ hours

How many transport calculations are needed for the KRUSTY uncertainty analysis (dimensions and positioning)?

- Central-difference formula for uncertainty in k due to parameter x_i: $u_{k,i} = \frac{\pm u_i}{2\delta x_i}\left[k_{eff}(x_{i,0}+\delta x_i) - k_{eff}(x_{i,0}-\delta x_i)\right]$
- Dimensions of each part: 2 × ~119 parts × 3–4= ~414–952
- Position of some components: ~2 × ~4 assemblies = ~8
- Gaps: 1 × ~80 places where there could be a gap = ~80
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Eigenvalue sensitivity to system dimensions

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MONTE CARLO CALCULATIONS OF EIGENVALUE SENSITIVITIES TO SYSTEM DIMENSIONS

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Data, Analysis, and Operations for Nuclear Criticality Safety—I

Adjoint-Based Eigenvalue Sensitivity to Geometry Perturbations, and a Warning

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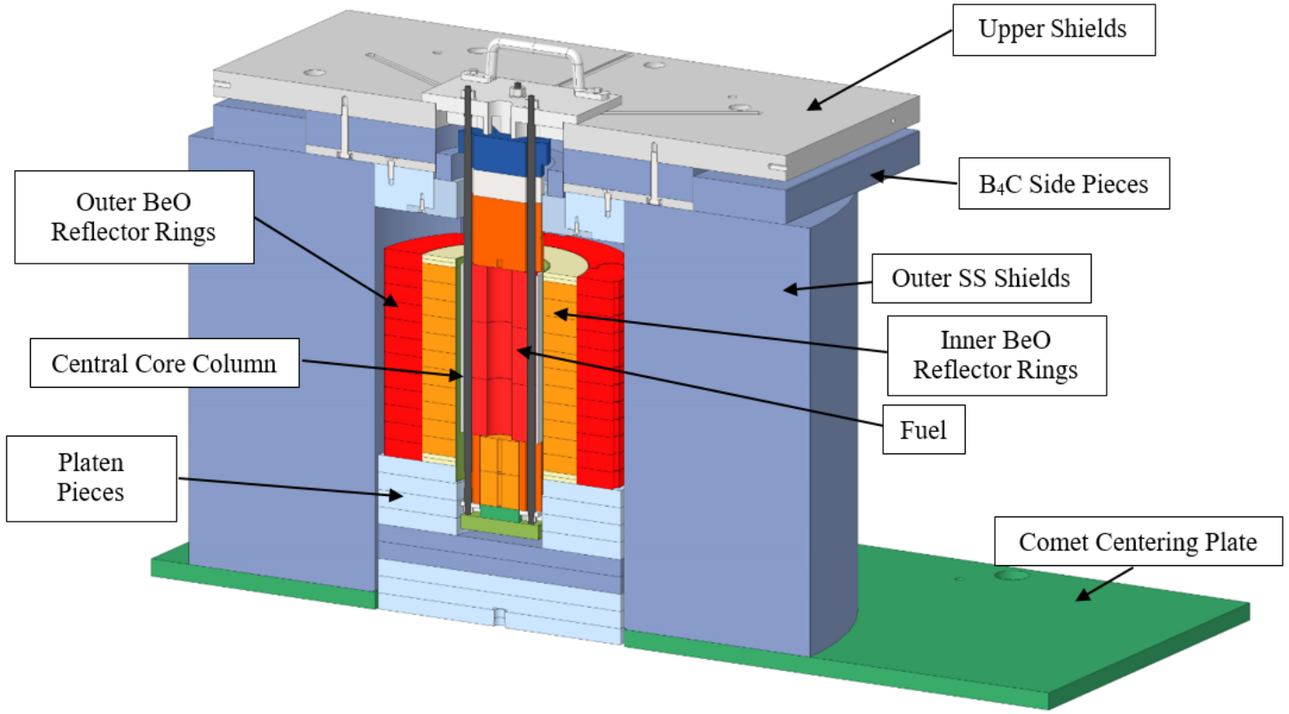
Largest Uncertainties for Case 3

Parameter	k_{eff} Combined Standard Uncertainty
Platen Radial Alignment	+ 0.00049 ± 3.33 %
Central Core Column Axial Alignment	± 0.00040 ± 3.21 %
Mass of Outer SS Shields	± 0.00029 ± 0.93 %
HEU Fuel Dimensions	± 0.00025 ± 1.23 %
Fuel Composition	± 0.00018 ± 0.34 %
Axial Central Core Column Gaps, Positive Contributions	+ 0.00017 ± 16.90 %
SS Outer Shields Composition	± 0.00009 ± 2.71 %
Axial Central Core Column Gaps, Negative Contributions	– 0.00008 ± 35.92 %
Other	± 0.00020 ± 6 %
Total	+ 0.00080 / – 0.00062 ± 2 %



- Representative of all five cases.
- Case 2 has an asymmetric contribution from the criticality measurement.

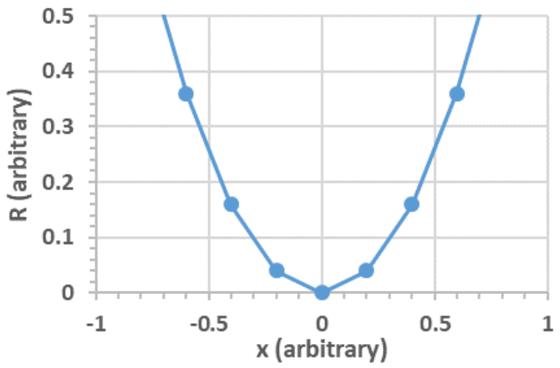
Platen Radial Alignment

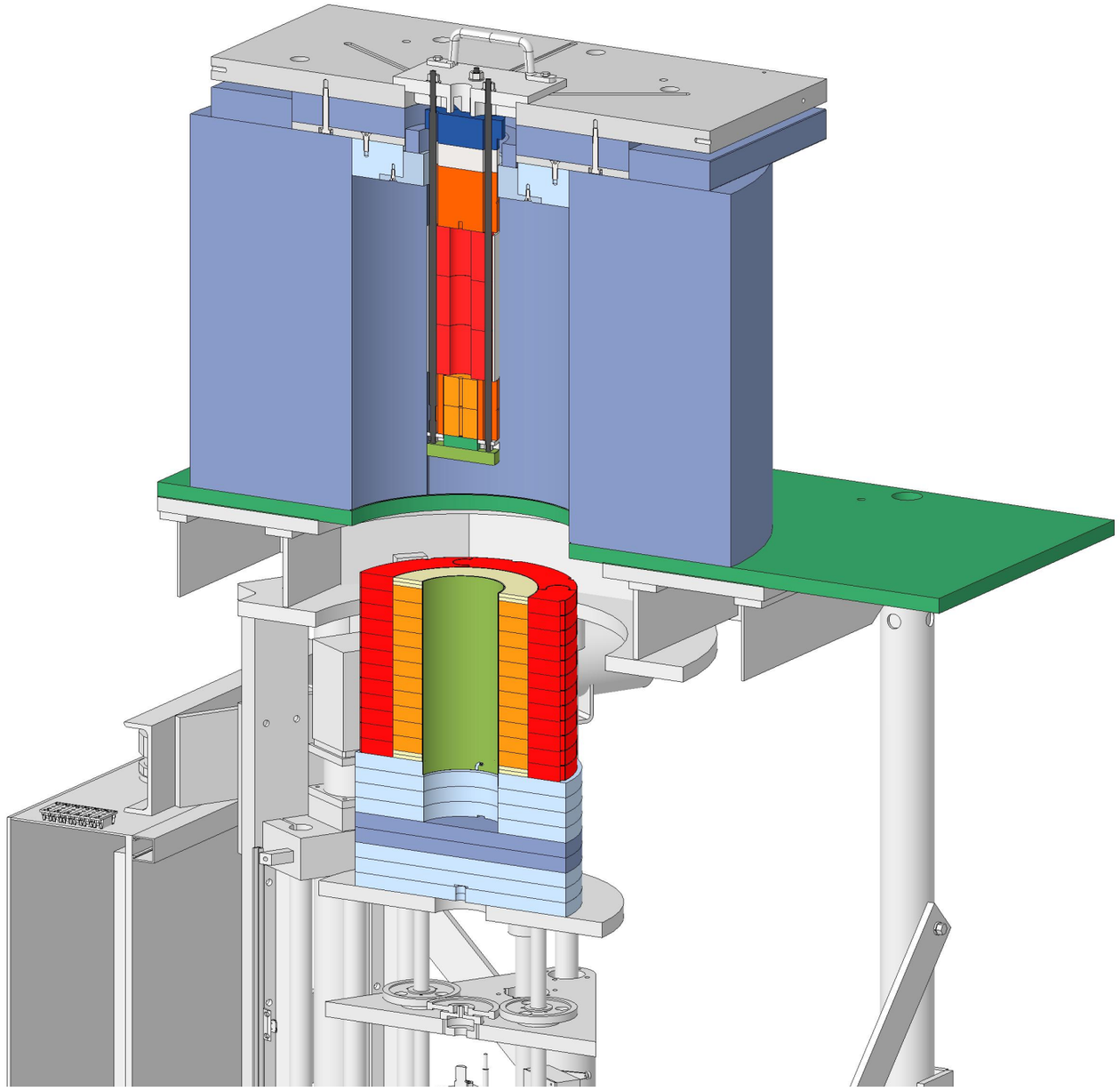
- The maximum (therefore bounding) platen radial misalignment, between the outer diameter of the platen plates and inner diameter of the Comet Centering Plate, was 0.25 in, in a single direction.

- For each case, the entire platen assembly (platen plates, BeO reflector rings, and Centering Ring) was offset from the center position by 0.25 inches in the direction parallel to the width of the Comet Centering Plate.

- The base case is centered; an offset in any direction leads to a larger k_{eff}.

  + What is the derivative at the base case?





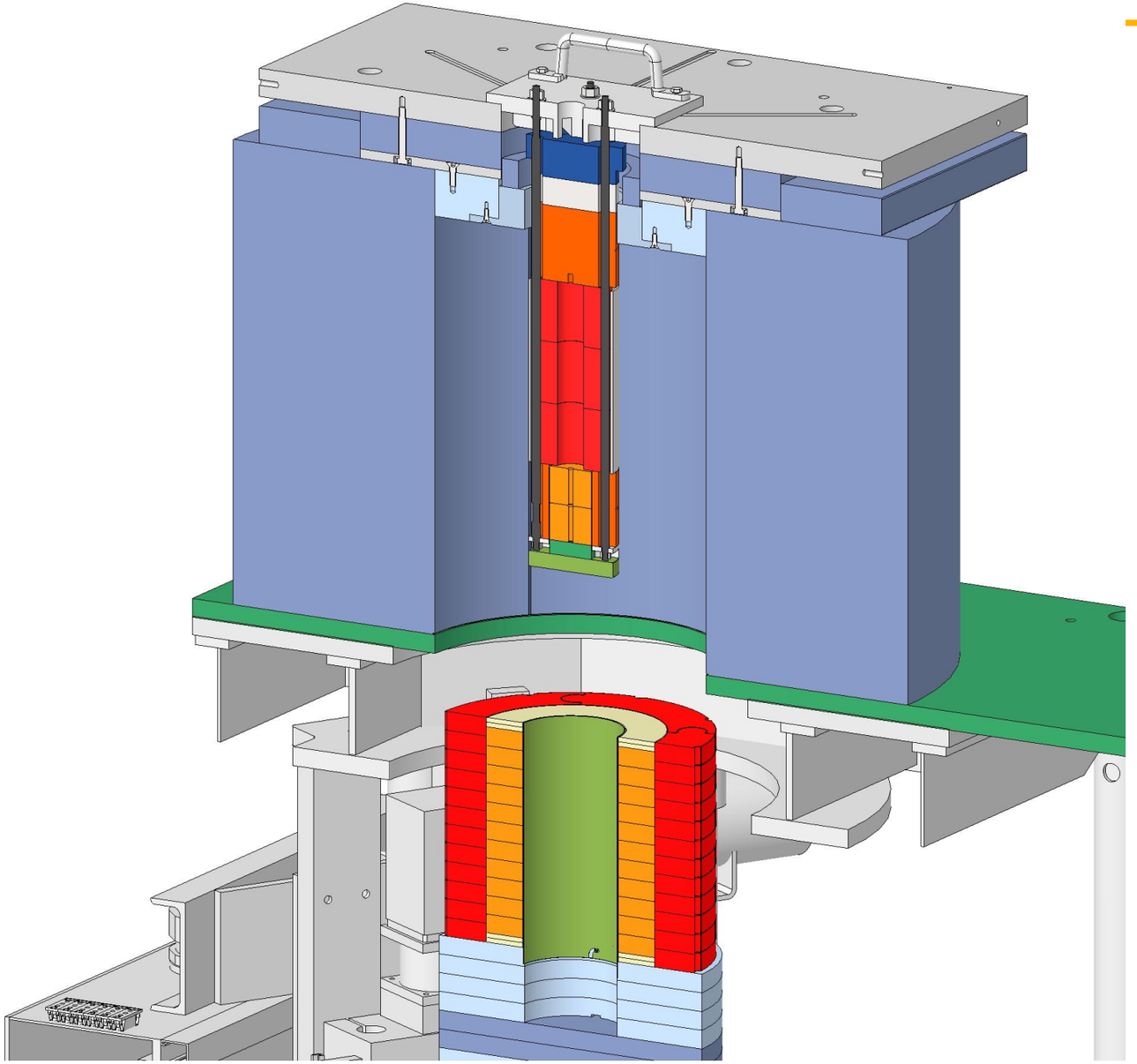
Central Core Column Axial Alignment

- The central core column is suspended from the top of the assembly.

- Its position depends on the uncertain heights and lengths of at least seven components.

- We added the uncertainty of each height or length in quadrature to obtain the uncertainty in the axial alignment of the central core column.

- In the perturbation calculations for the seven components, the location of the central core column was not perturbed.
  - + The length of the Support Rods was perturbed to preserve the location of the Central Core Column with respect to the BeO Shield.



Axial Central Core Column Gaps

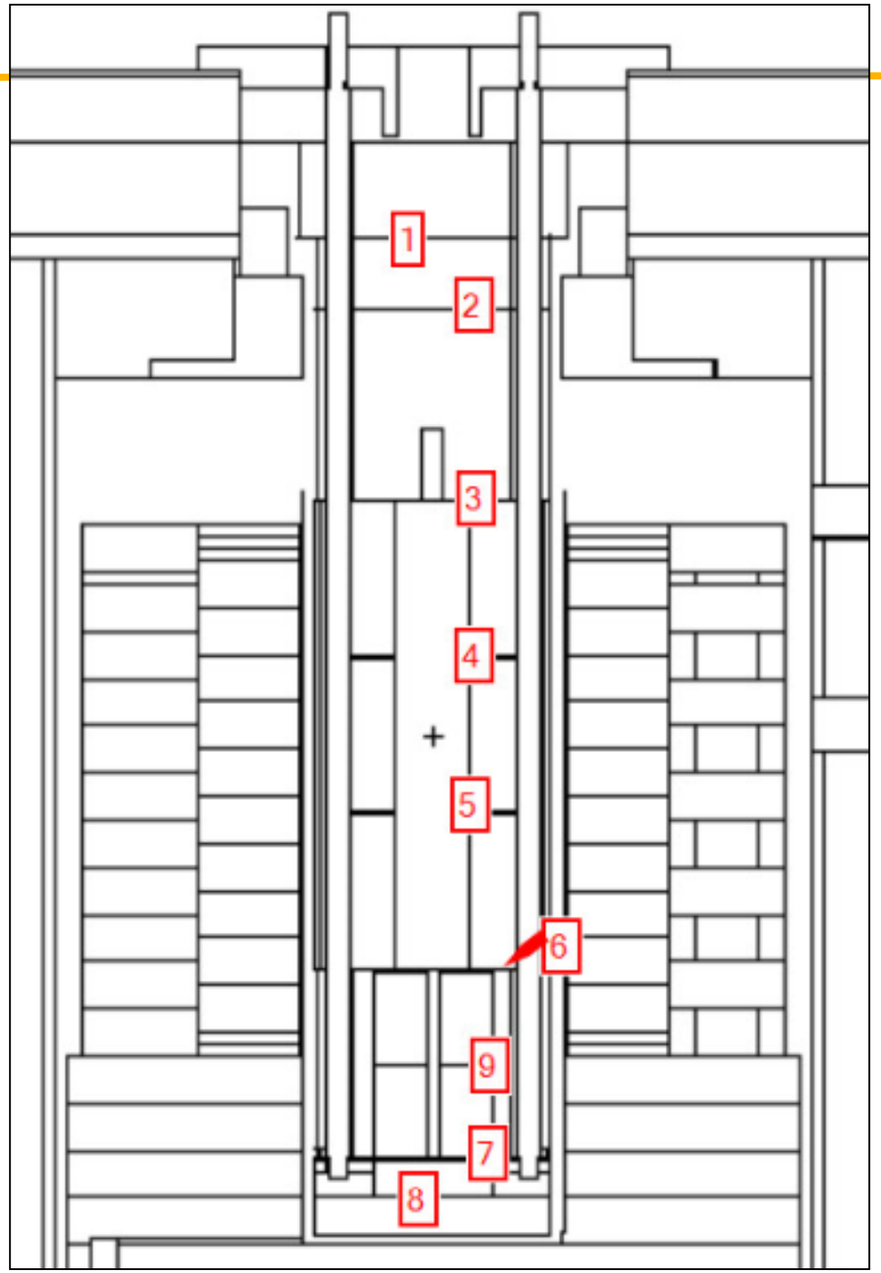
- It was assumed that the total gap which could potentially be caused by a component was the sum of the maximum flatness and maximum parallelism of the component.

- The bounding gap thickness was the sum of the potential gap caused by each of the two components at each interface.

- Introducing a gap causes a one-sided uncertainty.

- Results for Case 3

Gap Number	Final u_k
1	+ 0.00013
2	+ 0.00010
3	+ 0.00003
4	– 0.00003
5	– 0.00004
6	– 0.00006
7a, 7b	Negligible
8	Negligible
9	Negligible



SS Outer Shields Mass and Composition

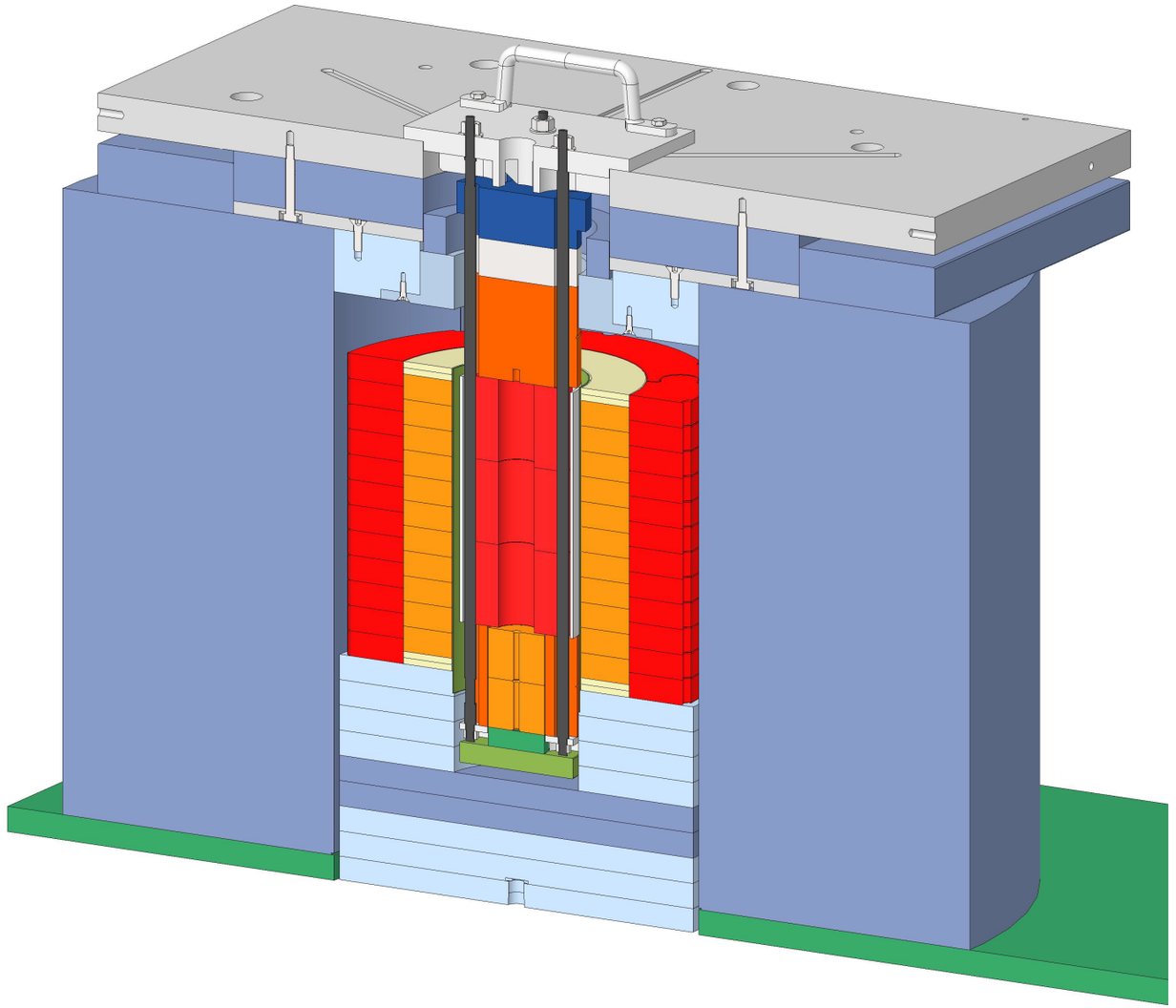
- The Outer SS Shields are enormous compared to the size of the core.

- As these components were too large for the scales available, the masses were not measured.

- A density of 8 g/cm^3 was assumed, and a large uncertainty of ± 1% was applied.

- The compositions were measured but uncertainties were not given, so again, a large uncertainty was applied.
  - ± 1% on the iron content,
  - ± 5% on chromium and nickel,
  - and ± 20% on all other impurities.

- The Outer SS Shields contributed about as much to the total uncertainty as the fuel did.



Fuel Dimensions

- The height is the most important dimension (for uncertainties).

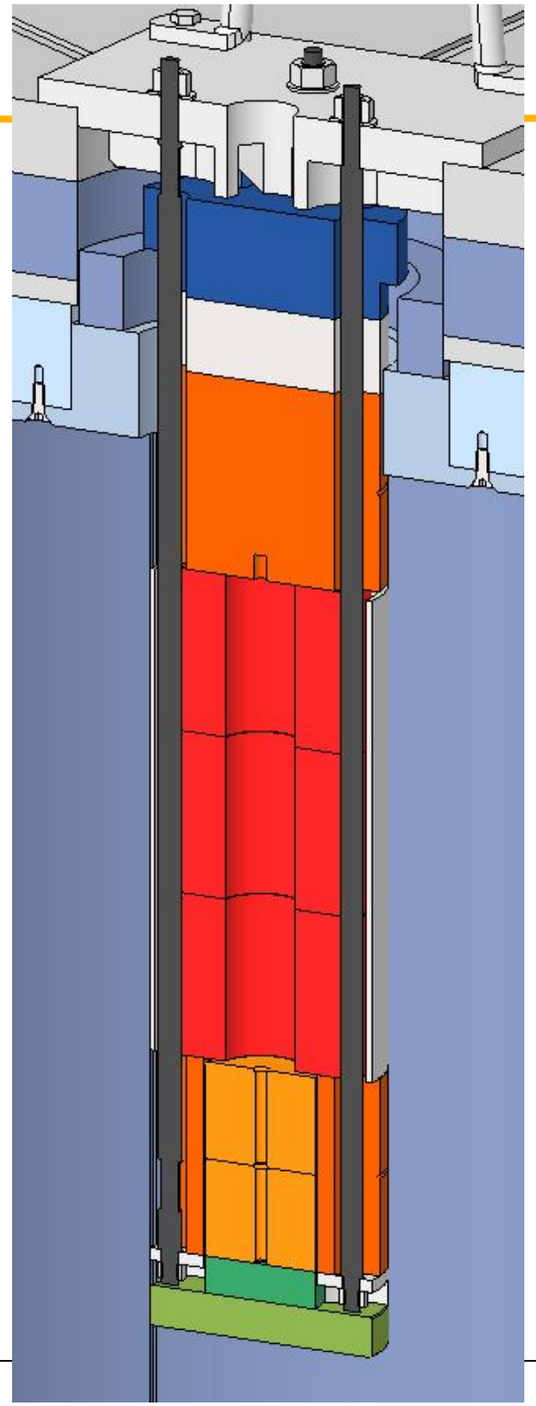
- What does it mean to perturb the height? One of these:
  - + the top surface of fuel element i is raised $\pm\Delta x_i$;
  - + the bottom surface of fuel element i is lowered $\pm\Delta x_i$;
  - + the top and bottom surfaces of fuel element i are both raised and lowered simultaneously by $\pm\Delta x_i/2$.

  - + In each case the heights of the other fuel elements were preserved by raising or lowering their top and bottom surfaces, but no other surfaces were perturbed.
  - + Fuel masses were preserved.

- Results for Case 3:

Component	Perturbed Surface	Final u_k
DAR2	Top	± 0.00014
	Bottom	± 0.00009
	Both	± 0.00012
DDND	Top	± 0.00017
	Bottom	± 0.00012
	Both	± 0.00014
D7XP	Top	± 0.00008
	Bottom	± 0.00003
	Both	± 0.00005

- u_k for the top surface was used as the uncertainty



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Fuel Composition

- For molybdenum, control parameter adjustment was used with uranium as the control parameter (or balance element), meaning that a change in the molybdenum concentration would be balanced by an equal and opposite change in the uranium concentration.

- For carbon, actinide impurities, and other impurities, control parameter adjustment was used with the U-Mo compound as the control parameter (or balance element), meaning that a change in the impurity concentration would be balanced by an equal and opposite change in the U-Mo concentration.

- For uranium isotopics except for U-232 and U-238, control parameter adjustment was used with U-238 as the control parameter, meaning that a change in a uranium isotope concentration would be balanced by an equal and opposite change in the U-238 concentration.

- For U-238, full normalization was used.

- The U-232 concentration was measured using gamma-ray spectroscopy, not ICP-MS, so full normalization was used for that isotope as well.

- Results for Case 3 for one fuel element:

Component	Nuclide	Final u_k
DDND	U-232	Negligible
	U-233	Negligible
	U-234	± 0.00003
	U-235	± 0.00002
	U-236	Negligible
	U-238	Negligible
	Mo	± 0.00012
	C	± 0.00001
	Actinides	Negligible
	Other	Negligible

- The uncertainty on the molybdenum was not provided. An uncertainty of ± 1000 ppm (0.1 wt%) was assumed to be bounding.

Benchmark Calculation Results for the Detailed Models

Code (Cross Section Set) → Case ↓	Benchmark	MCNP6.2 (Continuous-Energy ENDF/B-VIII.0)	
	k_{eff}	k_{eff}	C – E (pcm)
1	1.00063 + 0.00078 / – 0.00062	1.00043 ± 0.00002	–20
2	1.00343 + 0.00078 / – 0.00062	1.00325 ± 0.00002	–18
3	1.00015 + 0.00080 / – 0.00062	1.00017 ± 0.00002	2
4	1.00046 + 0.00076 / – 0.00060	1.00033 ± 0.00002	–13
5	1.00187 + 0.00076 / – 0.00059	1.00174 ± 0.00002	–13

Summary

- MCNP results for k_{eff} matched the measurements extremely well.
- The evaluated uncertainties are
  + Asymmetric
  + Smaller than 0.00100 (e.g. + 0.00080 / – 0.00062)
- The largest uncertainties are due to alignment.